Quasi-particle excitations and dynamical structure function of trapped Bose-condensates in the WKB approximation

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The Bogoliubov equations of the quasi-particle excitations in a weakly interacting trapped Bose-condensate are solved in the WKB approximation in an isotropic harmonic trap, determining the discrete quasi-particle energies and wave functions by torus (Bohr-Sommerfeld) quantization of the integrable classical quasi-particle dynamics. The results are used to calculate the position and strengths of the peaks in the dynamic structure function which can be observed by off-resonance inelastic light-scattering.

I. INTRODUCTION

The experimental realization of Bose-Einstein condensates of weakly interacting alkali atoms confined by magnetic traps [1–4] has revived the interest in the properties of Bose-condensed systems [5], in particular in solutions of the Gross-Pitaevski [6] equation in an external potential, describing the condensate, and of the Bogoliubov equations governing the quasi-particle excitations out of the spatially inhomogeneous condensate [7–9]. Approximate spatially inhomogeneous solutions of the Gross-Pitaevski equation have been obtained by a Gaussian variational ansatz, which is appropriate for moderate size condensates, and by the Thomas-Fermi approximation [10], which is very good for large condensates, except in a narrow region around the surface of the condensate. Similarly, solutions of the Bogoliubov equations for the low-lying quasi-particle excitations have been constructed numerically [7], by a variational method [8], and in the hydrodynamic limit [9]. Such low-lying states have recently been excited by resonant periodic variations in the trap parameters [11–13], and good agreement with the theoretical predictions has been obtained.

Much less work has been done so far on the high lying excitations, where all the methods which have so far been used for the low lying ones are either impracticable or don't apply. Such high lying states are of experimental interest because they are excited by off-resonance inelastic light scattering. In a previous paper [14] we have computed the high-lying quasi-particle energies and the amplitude of the inelastic peaks in the scattering function using the Thomas-Fermi approximation and solving the Hartree-Fock-Bogoliubov equations in perturbation theory of first order for the energies (with an estimate of the second order ones) but only to zero order in the wave functions. It is desirable to improve on this highly simplified approach by developing a self-consistent non-perturbative approach and extend the calculation to the whole energy region. It is our purpose, in the present paper, to present a non-perturbative method — the WKB approximation — for the solution of the Bogoliubov equations in a trap which allows us to interpolate between the hydrodynamical and the high-energy regime, and to use it to calculate the energies and wave-functions of the quasi-particle states. In a previous brief report we have already presented some results of our calculation of the high lying levels of the quasi-particles [15]. Here we shall apply our results to calculate the dynamical structure function, which is of high interest, because it could be measured in off-resonance light scattering [16–18]. Calculations of the dynamical structure function have previously been presented for the homogeneous ideal Bose gas [18,19] and for the homogeneous interacting Bose gas [20], which are however not directly applicable to the trapped condensates. Results have also been presented for the hydrodynamic limit of the structure function [21]. Very recently results for the dynamical structure function in the local density approximation have been presented [22], However, due to the limitations of that approximation, the resulting structure function cannot show structure beyond the constraints imposed by the locally averaged energy and momentum conservation.

The results we shall present here are applicable in a large enery domain ranging from low lying to high lying levels of the trapped condensates and retain the full information on the discrete nature of the quasi-particle levels. They are,however, restricted to the spatially isotropic case. In previous work [14] we have calculated the dynamical structure function for the very high lying quasiparticle levels in isotropic trapped condensates in a simpler approximation,

replacing the high lying states by free trap states. The more sophisticated non-perturbative calculation presented in the present paper shows, however, that the interaction of the high lying states with the condensate has a non-negligible influence on the selection of the angular momentum of the states excited by light-scattering.

An essential and independent input for our WKB-calculations is the condensate wave-function, which must be obtained by solving the Gross-Pitaevski equation. As we intend to carry out the WKB calculations analytically, as far as possible, we shall use here the main analytical approximation for large Bose-condensates with repulsive interaction, the Thomas-Fermi approximation. The necessary results are collected in section II.

In section III. the WKB approximation for the Boguliubov equations in an isotropic harmonic trap is developed. It is implemented in section IV. by studying the classical quasi-particle dynamics, which is integrable in isotropic traps. For a discussion of the non-integrable quasi-particle dynamics in anisotropic traps see [23].

The reduced action is calculated as a function of energy and angular momentum. In section IV. the Bohr-Sommerfeld quantization of the energy levels of the classical quasi-particle dynamics is performed and the semiclassical wave functions, properly normalized, are obtained in section V. The necessary integrals, though tedious, can all be done analytically.

In section VI. we present our results for the scattering function and in section VII some numerical examples are given. Our conclusions are summarized in the final section VIII.

II. BASIC EQUATIONS FOR CONDENSATE AND QUASI-PARTICLE EXCITATIONS

A necessary prerequisite of any calculation of the quasi-particle excitations is an appropriate description of the condensate. The relevant results are summarized in the present section. For weakly interacting atoms at zero temperature practically all particles are in the condensate and the energy E is a functional of the macroscopic condensate wave function $\psi_0(\boldsymbol{r})$

$$E(\{\psi_0\}) = \int d^2r \left[\frac{\hbar^2}{2m} |\boldsymbol{\nabla}\psi_0(\boldsymbol{r})|^2 + U(\boldsymbol{r})|\psi_0(\boldsymbol{r})|^2 + \frac{2\pi\hbar^2 a}{m} |\psi_0(\boldsymbol{r})|^4 \right] \tag{2.1}$$

where the constraint

$$\int d^3r |\psi_0(\boldsymbol{r})|^2 = N_0 \tag{2.2}$$

must be imposed. $U(\boldsymbol{r})$ is the trap potential. In our calculations we shall assume an isotropic harmonic trap

$$U(r) = \frac{1}{2} m\omega_0^2 r^2 \tag{2.3}$$

for simplicity. The scattering length is assumed to be positive and is denoted by a. The number of atoms in the condensate is denoted by N_0. We assume that the interaction is very weak and the temperature is close to zero, so that $N_0 \approx N$. The minimization condition for E, introducing the chemical potential μ as a Lagrange multiplier to enforce the constraint (2.2), yields the Gross-Pitaevski equation [6]

$$-\frac{\hbar^2}{2m} \nabla^2 \psi_0 + U(\boldsymbol{r})\psi_0 + \frac{4\pi\hbar^2 a}{m} |\psi_0|^2 \psi_0 = \mu\psi_0 \,. \tag{2.4}$$

A. Thomas-Fermi approximation

In the present paper we shall use as an analytical approximation for the minimum of (2.1) the Thomas Fermi approximation, which holds in the limit of large condensates $N_0 a >> d_0 \equiv \sqrt{\frac{\hbar}{m\omega_0}}$. In that limit it becomes a very good approximation to solve (2.4) by neglecting the kinetic energy term [10]

$$\psi_0(r) = \left(\frac{m}{4\pi\hbar^2 a} (\mu - U(r)) \right)^{1/2} \Theta(\mu - U(r)) \tag{2.5}$$

where μ must be determined as a function of N_0 by imposing the normalization condition (2.2), which yields

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$$\mu = \frac{\hbar\omega_0}{2}(15N_0a/d_0)^{2/5} \tag{2.6}$$

The conditions $\mu >> \hbar\omega_0$ and $N_0a >> d_0$ are therefore equivalent. In eq. (2.5) $\Theta(x)$ is the step function. The approximation eq. (2.5) with discontinuous derivative at $r = r_0 = \sqrt{2\mu/m\omega_0^2}$ is sufficient, except in those cases where derivatives of the wave-function $\psi_0(r)$ for r close to r_0 are important. In the latter case a boundary layer theory can be used to compute the condensate wave function close to the Thomas Fermi radius [24], but we shall not need this improvement in the present paper.

B. Quasi-particle excitations

Let us now turn to a Bose condensate with excitations and adopt a description in the Heisenberg picture, where the field operator satisfies the equation of motion

$$i\hbar\frac{\partial\hat{\psi}}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\hat{\psi} + U(\boldsymbol{r})\hat{\psi} + \frac{4\pi\hbar^2 a}{m}\hat{\psi}^+\hat{\psi}\hat{\psi}\,. \tag{2.7}$$

For a weakly interacting Bose condensed gas the Bogoliubov approximation consists in splitting the total Bose field operator $\hat{\psi}(t)$ into

$$\hat{\psi}(t) = (\psi_0 + \hat{\phi}(t))e^{-i\mu t/\hbar}\,, \tag{2.8}$$

where ψ is the time-independent condensate wave function and $\hat{\phi}(t)$ describes the excitations from the condensate, and to linearize the field equation for $\hat{\phi}(t)$

$$i\hbar\frac{\partial\hat{\phi}}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + U(\boldsymbol{r}) - \mu + \frac{8\pi\hbar^2 a}{m}|\psi_0(\boldsymbol{r})|^2\right)\hat{\phi} + \frac{4\pi\hbar^2 a}{m}\psi_0(\boldsymbol{r})^2\hat{\phi}^+\,. \tag{2.9}$$

The Bogoliubov transformation

$$\hat{\phi}(t) = \sum_j{}' \left(u_j(\boldsymbol{r})\alpha_j e^{-i\omega_j t} - v_j^*(\boldsymbol{r})\alpha_j^+ e^{i\omega_j t}\right) \tag{2.10}$$

and its adjoint, with Bose operators α_j, α_j^+ for the quasi-particle excitations and with the sum over j restricted to states with $\omega_j \neq 0$, yields the Bogoliubov equations

$$\begin{pmatrix} -\frac{\hbar^2}{2m}\nabla^2 + U_{\text{eff}}(\boldsymbol{r}) - E_j & -K(\boldsymbol{r}) \\ -K^*(\boldsymbol{r}) & -\frac{\hbar^2}{2m}\nabla^2 + U_{\text{eff}}(\boldsymbol{r}) + E_j \end{pmatrix}\begin{pmatrix} u_j \\ v_j \end{pmatrix} = 0, \tag{2.11}$$

where we used the abbreviations

$$E_j = \hbar\omega_j \quad, \quad U_{\text{eff}}(\boldsymbol{r}) = U(\boldsymbol{r}) + \frac{8\pi\hbar^2 a}{m}|\psi_0(\boldsymbol{r})|^2 - \mu$$

$$K(\boldsymbol{r}) = \frac{4\pi\hbar^2 a}{m}\psi_0(\boldsymbol{r})^2\,. \tag{2.12}$$

Eq. (2.11) is consistent with and its solutions must be chosen to satisfy the orthonormality conditions

$$\int d^3r(u_j u_k^* - v_j v_k^*) = \delta_{jk}$$

$$\int d^3r(u_j^* v_k - u_k^* v_j) = 0 \tag{2.13}$$

in order to guarantee the Bose commutation relations of the α_j, α_j^+.

A formal solution of eq. (2.11) at zero energy $E_j = 0$ is given by the condensate

$$u_j = v_j^* = \psi_0(\boldsymbol{r}) \quad, \quad E_j = 0\,, \tag{2.14}$$

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but this solution is not normalizable in the required sense. For a harmonic trap $U(\boldsymbol{r}) = \frac{1}{2}m\sum_{i=1}^{3}\omega_{0i}^2 x_i^2$ three linearly independent and correctly normalized exact solutions

$$u_i = b_i^+ \psi_0(\boldsymbol{r}) \quad , \quad v_i = b_i \psi_0^*(\boldsymbol{r}) \quad , \quad E_i = \hbar\omega_{0i} \tag{2.15}$$

always exist [25], where

$$b_i = \sqrt{\frac{\hbar}{2m\omega_{0i}}}\frac{\partial}{\partial x_i} + \sqrt{\frac{m\omega_{0i}}{2\hbar}}x_i \quad , \quad b_i^+ = (b_i)^+ \tag{2.16}$$

are the Bose operators for the harmonical oscillations in the trap.

III. WKB-APPROXIMATION FOR QUASI-PARTICLE STATES IN THE CLASSICALLY ALLOWED REGION

We shall here treat the WKB approximation for the case of an isotropic harmonic trap, where $U_{\text{eff}}(r)$ and $K(r)$ depend only on the radial coordinate r.

Let us drop the index j for the time being and expand formally in $\hbar$

$$u = (a_0(r) + \hbar a_1(r) + \hbar^2 a_2(r) + \ldots)e^{iS(r)/\hbar}Y_{lm}(\theta,\phi)$$
$$v = (b_0(r) + \hbar b_1(r) + \hbar^2 b_2(r) + \ldots)e^{iS(r)/\hbar}Y_{lm}(\theta,\phi). \tag{3.1}$$

In Eq. (3.1) we shall treat $U_{\text{eff}}(r)$ and $K(r)$ as being independent of $\hbar$. The angular dependence is separated out by the spherical harmonics Y_{lm}. The angular momentum, denoted by J in the following, is then quantized in the usual way by $J^2 = \hbar^2 l(l+1)$, which will be replaced in our WKB-treatment according to Langer's rule $J^2 = \hbar^2(l+1/2)^2$. Inserting the ansatz (3.1) into (2.11) we obtain up to order $\hbar^2$ the equations

$$\boldsymbol{L}_0\begin{pmatrix}a_0\\b_0\end{pmatrix} = 0 \tag{3.2}$$

$$\boldsymbol{L}_0\begin{pmatrix}a_1\\b_1\end{pmatrix} = -\boldsymbol{L}_1\begin{pmatrix}a_0\\b_0\end{pmatrix} \tag{3.3}$$

$$\boldsymbol{L}_0\begin{pmatrix}a_2\\b_2\end{pmatrix} = -\boldsymbol{L}_1\begin{pmatrix}a_1\\b_1\end{pmatrix} - \boldsymbol{L}_2\begin{pmatrix}a_0\\b_0\end{pmatrix} \tag{3.4}$$

with

$$\boldsymbol{L}_0 = \begin{pmatrix} \frac{p_r^2}{2m} + \frac{J^2}{2mr^2} + U_{\text{eff}}(r) - E & -K(r) \\ -K^*(r) & \frac{p_r^2}{2m} + \frac{J^2}{2mr^2} + U_{\text{eff}}(r) + E \end{pmatrix} \tag{3.5}$$

$$\boldsymbol{L}_1 = -\frac{i}{m}\left(p_r\frac{d}{dr} + \frac{1}{2}\frac{dp_r}{dr} + \frac{p_r}{r}\right)\begin{pmatrix}1&0\\0&1\end{pmatrix} \tag{3.6}$$

$$\boldsymbol{L}_2 = -\frac{1}{2m}(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr})\begin{pmatrix}1&0\\0&1\end{pmatrix} \tag{3.7}$$

where $p_r = dS/dr$.

The solvability condition of (3.2), the vanishing of the determinant of L_0, gives the condition

$$\det(\boldsymbol{L}_0) = \left(\frac{1}{2m}\left(\frac{dS}{dr}\right)^2 + \frac{J^2}{2mr^2} + U_{\text{eff}}(r)\right)^2 - E^2 - |K(r)|^2 = 0. \tag{3.8}$$

We can solve this equation for E, restricting ourselves to the branch $E > 0$, because the replacement $E \to -E$ merely amounts to the renaming $u \to v^*$, $v \to u^*$. Then we obtain the time-independent Hamilton-Jacobi equation

$$H(dS/dr, r) = E \tag{3.9}$$

with

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$$H(p_r, r) = \sqrt{\left(\frac{p_r^2}{2m} + \frac{J^2}{2mr^2} + U_{\text{eff}}(r)\right)^2 - |K(r)|^2}\,. \tag{3.10}$$

This defines the Hamiltonian for the classical quasi-particle dynamics. Introducing the time-dependent action

$$W(r, t) = S(r) - Et \tag{3.11}$$

we may replace eq. (3.9) by the time-dependent Hamilton Jacobi equation

$$\frac{\partial W}{\partial t} + H\left(\frac{\partial W}{\partial r}, r\right) = 0\,. \tag{3.12}$$

It follows from eq. (3.8) that with S also $-S$ is a solution of the Hamilton Jacobi equation (3.9). It is interesting to note that the classical quasi-particle dynamics is integrable only in the special case of an isotropic harmonic trap. Even in the experimentally realized case of an anisotropic axially symmetric trap the classical quasi-particle dynamics turns out to be nonintegrable, in general. A detailed investigation is given in [23]. In this case a semi-classical quantization of the quasi-particle dynamics requires the methods introduced in the field of quantum chaos, such as semiclassical quantization based on periodic orbits, or even replacing the quasi-particle spectrum and wave-functions by results based on random matrix theory.

After satisfying eq. (3.8) the general solution of eq. (3.2) can be written in the form

$$\begin{pmatrix} a_0 \\ b_0 \end{pmatrix} = a_0(r) \begin{pmatrix} 1 \\ \frac{-E + \sqrt{E^2 + |K(r)|^2}}{K(r)} \end{pmatrix} \tag{3.13}$$

where $a_0(r)$ is still arbitrary.

$\boldsymbol{L}_0$ is not invertible. The solvability condition of eq. (3.3) is that its inhomogeneity is orthogonal to the kernel of $\boldsymbol{L}_0$

$$(a_0^*, b_0^*)\boldsymbol{L}_1 \begin{pmatrix} a_0 \\ b_0 \end{pmatrix} = 0\,. \tag{3.14}$$

Evaluating this condition for $a_0(r) \neq 0$ we obtain after some rearrangements a classical transport equation for a_0,

$$\frac{dS}{dr}\frac{d}{dr} \ln\left(|a_0(r)|^2 \left(1 + (\sqrt{1 + E^2/|K(r)|^2} - E/|K(r)|)^2\right)\right) + \frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{dS}{dr}\right) = 0, \tag{3.15}$$

which can be rewritten as a continuity equation

$$\frac{1}{r^2}\frac{d}{dr}\left[r^2 |a_0(r)|^2 \left(1 + \left(\sqrt{1 + E^2/|K(r)|^2} - E/|K(r)|\right)^2\right)\frac{dS}{dr}\right] = 0\,. \tag{3.16}$$

The physical meaning of this result as classical conservation law for the quasi-particle current becomes clear if we rewrite it once more as

$$\frac{1}{r^2}\frac{d}{dr}\left[r^2 \left(|a_0(r)|^2 - |b_0(r)|^2\right) v_r(r)\right] = 0, \tag{3.17}$$

where we used the identities

$$v_r(r) \equiv \left(\frac{\partial}{\partial p_r}H(p_r, r)\right)_{p_r = dS/dr} = \frac{\sqrt{E^2 + |K(r)|^2}}{E}\frac{1}{m}\frac{dS}{dr} = \frac{1}{m}\frac{|K|^2 + (\sqrt{E^2 + |K|^2} - E)^2}{|K|^2 - (\sqrt{E^2 + |K|^2} - E)^2}\frac{dS}{dr} \tag{3.18}$$

to express dS/dr in terms of the radial component $v_r(r)$ of the quasi-particle velocity field. The general solution of eq. (3.17) can therefore be written as

$$|a_0|^2 - |b_0|^2 = \frac{const}{r^2 v_r(r)} \tag{3.19}$$

In principle, this procedure can be continued. Having satisfied the solvability condition for eq. (3.3) we can determine its general solution in the form

$$\begin{pmatrix} a_1 \\ b_1 \end{pmatrix} = a_1(r) \begin{pmatrix} 1 \\ -E/|K| + \sqrt{1 + E^2/|K|^2} \end{pmatrix} + \begin{pmatrix} 0 \\ b_1^{\mathrm{part}}(r) \end{pmatrix}. \tag{3.20}$$

Here the first term is the general solution of the homogeneous equation whose still arbitrary amplitude $a_1(r)$ must be determined from the solvability condition of eq. (3.4)

$$(a_0^*, b_0^*) \left\{ \boldsymbol{L}_1 \begin{pmatrix} a_1 \\ b_1 \end{pmatrix} + \boldsymbol{L}_0 \begin{pmatrix} a_0 \\ b_0 \end{pmatrix} \right\} = 0. \tag{3.21}$$

The second term in eq. (3.20) is a particular solution of eq. (3.3), which we choose with vanishing amplitude $a_1^{\mathrm{part}}(r) = 0$ in order to define the first term in eq. (3.20) in an unambiguous way. As we shall not need the explicit form of a_1, b_1 we shall here not work it out from eqs. (3.20), (3.21).

IV. SEMICLASSICAL QUASI-PARTICLE ENERGIES IN ISOTROPIC HARMONIC TRAPS

For the radial canonical momentum as a function of r we obtain from (3.10)

$$p_r = \sqrt{2m} \sqrt{\sqrt{E^2 + K^2(r)} - \frac{J^2}{2mr^2} - U_{\mathrm{eff}}(r)}. \tag{4.1}$$

The semi-classical quantization can now be performed in a straightforward manner by putting for the angular momentum

$$J = J_\ell = \hbar(\ell + 1/2) \tag{4.2}$$

and for the radial action variable

$$I_r(E, J) = \frac{1}{\pi} \int_{r_<}^{r_>} p_r(E, J, r) dr = \hbar(n_r + 1/2). \tag{4.3}$$

Here ℓ, n_r are the integer angular momentum and radial quantum number, respectively. We used 'Langer's rule' [26] of semi-classical angular momentum quantization by including $1/2$ on the right hand side of (4.2), and took into account a phase-shift of $\pi/4$ in the wave function at the classical turning points $r_<$, $r_>$ of the radial motion by including $1/2$ on the right hand side of (4.3).

For the Thomas Fermi approximation of the condensate the radial integral in eq. (4.3) can be performed analytically, even though the resulting expressions become rather lengthy. In this manner an implicit analytical formula for the energy levels in WKB approximation is obtained. Numerically solving the implicit expression for E for different values of n_r, ℓ we obtain the energy levels $E_{n_r l}$ in WKB approximation.

A. Types of motion

In Thomas-Fermi approximation (2.5) we have

$$U_{\mathrm{eff}}(r) = \left| \mu - \frac{m}{2}\omega_0^2 r^2 \right|$$
$$K^2(r) = \left(\mu - \frac{m}{2}\omega_0^2 r^2 \right)^2 \Theta \left(\mu - \frac{m}{2}\omega_0^2 r^2 \right) \tag{4.4}$$

where

$$\mu = \frac{\hbar\omega_0}{2} R_0^2 \quad,$$
$$R_0 = \left(\frac{15 N_0 a}{d_0} \right)^{1/5} = \frac{r_0}{d_0}, \quad d_0 = \sqrt{\frac{\hbar}{m\omega_0}}. \tag{4.5}$$

The Thomas-Fermi approximation requires $R_0^2 \gg 1$ for consistency. Let us introduce scaled variables and parameters by

$$\rho = (r/d_0 R_0) \quad , \quad \epsilon = E/\mu \quad , \quad j = (J/\hbar R_0^2) \quad , \quad \pi_r = p_r(d_0/\hbar R_0) \,. \tag{4.6}$$

Then eq. (4.1) becomes

$$\pi_r = \sqrt{\sqrt{\epsilon^2 + (1 - \rho^2)^2 \Theta(1 - \rho)} - j^2/\rho^2 - |1 - \rho^2|} \,. \tag{4.7}$$

In order to find the turning points $\rho_<$, $\rho_>$ we have to look for the solutions of $\pi_r = 0$.
i) Domain $\rho < 1$: Turning points in this region have to satisfy

$$\rho_<^2 = \frac{j^2}{\epsilon^2 + 2j^2} \left(1 + \sqrt{1 + \epsilon^2 + 2j^2} \right) \,. \tag{4.8}$$

The negative root is dismissed because only real and positive solutions are physical. The remaining solution (4.8) turns out to be a lower boundary of the ρ-values for which π_r is real. The condition

$$\rho_<^2 < 1 \qquad \text{(type B motion)} \tag{4.9}$$

is only fulfilled if

$$\epsilon > j^2 \qquad \text{(type B motion)} \,. \tag{4.10}$$

We shall denote this motion as being of type B. As there is only a lower turning point $\rho_<$ within the region $\rho < 1$, the upper turning point must lie in the region $\rho > 1$, i.e. for type B motion the quasi-particle leaves and reenters the condensate during each radial period.
ii) Domain $\rho > 1$: Turning points in this region must satisfy

$$\left. \begin{array}{c} \rho_> \\ \rho_< \end{array} \right\} = \frac{1}{2}(\epsilon + 1) \pm \frac{1}{2} \sqrt{(\epsilon + 1)^2 - 4j^2} \,. \tag{4.11}$$

They exist if and only if

$$\epsilon \geq 2j - 1 \tag{4.12}$$

where we recall that ϵ is restricted to $\epsilon > 0$ by definition. The lower turning point given by eq. (4.11) exists only if it satisfies

$$\rho_<^2 > 1 \qquad \text{(type A motion)} \tag{4.13}$$

in which case the classical quasi-particle dynamics is entirely confined to the region outside the condensate. It is then simply the motion in the harmonic potential of the trap. We call this motion being of type A. It requires the conditions

$$\epsilon > 1 \quad , \quad j^2 > \epsilon \quad > \quad 2j - 1 \quad \text{(type A motion)} \tag{4.14}$$

all to be satisfied, see fig. 1.
   If the turning point $\rho_<$ does not exist in the region $\rho > 1$, then the turning point $\rho_<$ must occur for $\rho < 1$, i.e. the only alternative of type A motion is motion of type B satisfying eqs. (4.9), (4.10). The upper turning point of both types of motion lies in the region $\rho > 1$ and is given by

$$\rho_>^2 = \frac{1}{2}(\epsilon + 1) + \frac{1}{2} \sqrt{(\epsilon + 1)^2 - 4j^2} \quad \text{(type A, B motion)} \,. \tag{4.15}$$

It is easily checked that $\rho_>^2 > 1$ for both types of motion. In fig. 1 the parts of the angular momentum — energy plane accessible to the two types of motion are shown. Let us now proceed to evaluate the radial action of both types of motion and quantize.

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B. Asymptotic limit of a large condensate $R_0 \to \infty$

The integral to be evaluated is

$$I_r = \frac{\hbar R_0^2}{\pi} \int_{\rho_<}^{\rho_>} \pi_r d\rho \,. \tag{4.16}$$

In order to obtain simple closed expressions we first study the case of a large condensate for which $R_0 \to \infty$, while we keep the energy E and angular momentum J of the quasi-particle fixed, i.e. the scaled quantities

$$\epsilon = \frac{2E}{\hbar\omega_0} \frac{1}{R_0^2} \quad , \quad j = \frac{\ell + 1/2}{R_0^2} \tag{4.17}$$

are both $0(R_0^{-2})$ in that limit. It follows that the necessary condition for type A motion $\epsilon \leq j^2$ (i.e. motion which remains outside the condensate) cannot be fulfilled in this limit, and therefore only type B motion can occur. In the present limit we have asymptotically

$$\rho_< \simeq \frac{\hbar\omega_0(\ell + 1/2)}{\sqrt{2E^2 + (\hbar\omega_0)^2(\ell + 1/2)^2}}, \quad \rho_> \simeq \sqrt{1 + \epsilon} \tag{4.18}$$

$$\pi_r \simeq \Theta(1 - \rho)\frac{1}{R_0^2}\sqrt{\frac{2E^2}{\hbar^2\omega_0^2}\frac{1}{(1 - \rho^2)} - \frac{(\ell + 1/2)^2}{\rho^2}} \tag{4.19}$$

$$+\Theta(\rho - 1)\sqrt{\epsilon + 1 - \rho^2} \,.$$

The integral

$$I_> = \frac{\hbar R_0^2}{\pi} \int_1^{\sqrt{1+\epsilon}} \sqrt{1 + \epsilon - \rho^2} d\rho \tag{4.20}$$

can be performed asymptotically for $\epsilon \to 0$ with the result

$$I_> = \frac{\hbar}{3\pi} \frac{1}{R_0} \left(\frac{2E}{\hbar\omega_0}\right)^{3/2} \to 0 \,. \tag{4.21}$$

The contribution of the part of the type B motion outside the condensate to the total radial action therefore becomes negligible $0(R_0^{-1})$ as $R_0 \to \infty$. The $0(1)$-part of the action is therefore given by

$$I_r \simeq \frac{\hbar}{\pi} \int_{\rho_<}^1 \sqrt{\frac{2E^2}{\hbar^2\omega_0^2}\frac{1}{(1 - \rho^2)} - \frac{\left(\ell + \frac{1}{2}\right)^2}{\rho^2}} d\rho \,. \tag{4.22}$$

The substitution

$$\rho^2 = 1 - \frac{E^2}{E^2 + (\ell + 1/2)^2(\hbar\omega_0)^2/2} \sin^2\varphi \tag{4.23}$$

reduces the integral to a rational function of $\sin\varphi$ and we obtain after integration

$$I_r = \frac{\hbar}{2}\left(\sqrt{2(E/\hbar\omega_0)^2 + (\ell + 1/2)^2} - (\ell + 1/2)\right) + 0\left(\frac{1}{R_0}\right) \,. \tag{4.24}$$

From the semi-classical quantization rule $I_r = \hbar(n_r + 1/2)$ we obtain the energy levels

$$E_{n_r\ell} = \hbar\omega_0(2n_r^2 + 2n_r\ell + 3n_r + \ell + 1)^{1/2}\left(1 + 0\left(\frac{1}{R_0}\right)\right) \,. \tag{4.25}$$

This result is remarkably close to the hydrodynamic result

$$E_{n_r\ell}^{\text{hyd}} = \hbar\omega_0(2n_r^2 + 2n_r\ell + 3n_r + \ell)^{1/2} \tag{4.26}$$

derived by Stringari [9] for the low lying levels in the hydrodynamic regime. In that regime the WKB-method is not applicable, but for energies $E_{n_r\ell} >> \hbar\omega_0$ the agreement between (4.25) and (4.26) becomes very good. Thus we find that there is a common regime of applicability of both the hydrodynamic approximation and the WKB approximation, where the energy is sufficiently large to apply the WKB approximation but not too large to invalidate the hydrodynamic approach.

C. Large-energy limit

For type A motion the classical particle never enters the condensate and the Bohr-quantization (4.3) leads to

$$E_{n_r\ell} = \hbar\omega_0(2n_r + \ell + 3/2) - \mu \equiv E_n^{osc}. \tag{4.27}$$

which depends only on the pricipal quantum number $n = 2n_r + \ell$ (see equation (4.35) below). However, for type B motion, i.e., $\epsilon \geq j^2$, $E_{n_r\ell}$ differs from $E_{n_r\ell}^{osc}$

$$E_{n_r\ell} = E_n^{osc} + \hbar\omega_0\delta_{n\ell}. \tag{4.28}$$

The shift $\delta_{n\ell}$ lifting the degenerecy of the free oscillator levels is expected to be small in the large-energy limit $E_{n_r\ell} \gg \mu$ and can be calculated in the following way:

For type B motion (4.3) can be written as

$$n_r + 1/2 = \frac{R_0^2}{\pi}\int_{\rho_<}^{\rho_>} \pi_r(\rho)\,d\rho = \frac{R_0^2}{\pi}\int_{\rho_<}^{1} d\rho\sqrt{\sqrt{\epsilon^2 + (1-\rho^2)^2} - j^2/\rho^2 - (1-\rho^2)}$$

$$+ \frac{R_0^2}{\pi}\int_{\rho_<^{(o)}}^{\rho_>} d\rho\sqrt{\epsilon^2 - j^2/\rho^2 + (1-\rho^2)} - \frac{R_0^2}{\pi}\int_{\rho_<^{(o)}}^{1} d\rho\sqrt{\epsilon^2 - j^2/\rho^2 + (1-\rho^2)}, \tag{4.29}$$

where $\rho_<^{(o)}$ and $\rho_>$ are the turning points for $\pi(\rho) = \sqrt{\epsilon^2 - j^2/\rho^2 + (1-\rho^2)}$, i.e., for the free oscillator:

$$\rho_>,\rho_<^{(o)} = \sqrt{\left(\frac{\epsilon+1}{2}\right) \pm \sqrt{\left(\frac{\epsilon+1}{2}\right)^2 - j^2}}. \tag{4.30}$$

The second integral in (4.29) is trivial and using (4.28) eq. (4.29) can be written as

$$\delta_n(\ell) = \frac{2R_0^2}{\pi}\int_{\rho_<}^{1} d\rho\sqrt{\sqrt{\epsilon^2 + (1-\rho^2)^2} - j^2/\rho^2 - (1-\rho^2)}$$

$$- \frac{2R_0^2}{\pi}\int_{\rho_<^{(o)}}^{1} d\rho\sqrt{\epsilon^2 - j^2/\rho^2 + (1-\rho^2)}. \tag{4.31}$$

For type B motion $j^2 \leq \epsilon$, thus in the present limit $\epsilon \to \infty$ and $a \equiv j^2/\epsilon$ is kept fixed ($0 \leq a \leq 1$). Our small parameter is $1/\epsilon$. In this limit the two integrals in leading order cancel each other. With the replacement $\rho^2 = 1 - z$ the next to leading approximation gives

$$\delta_n(\ell) = \frac{R_0^2}{\pi\sqrt{\epsilon}}\int_0^{1-a} dz\frac{z}{\sqrt{1-z-a}} = \frac{4R_0^2}{3\pi\sqrt{\epsilon}}(1-a)^{3/2}. \tag{4.32}$$

The shift is clearly tending to zero in the large energy limit, thus one can replace the unscaled energy $E_{n_r\ell}$ with E_n^{osc} on the right hand side of eq. (4.32):

$$\delta_n(\ell) = \frac{1}{3\pi}\frac{\left[(4\mu/\hbar\omega_0)(n+3/2 - \mu/\hbar\omega_0) - (\ell+1/2)^2)\right]^{3/2}}{\left[n+3/2 - \mu/\hbar\omega_0\right]^2}, \tag{4.33}$$

which is the asymptotics of the shift in the large energy limit. This is the result presented in [15]. For large values of $n = 2n_r + 2\ell$ it agrees with the perturbative result of [14].

D. Radial action in the case of a finite condensate

We now evaluate the radial action for finite R_0. The two types of motion must be considered separately.

Type A motion:
This type of motion requires $1 \leq 2j - 1 \leq \epsilon \leq j^2$. Its radial action is that of the free harmonic trap and easily obtained as

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$$I_r(\epsilon, j) = \frac{\hbar R_0^2}{\pi} \int_{\rho_<}^{\rho_>} \frac{d\rho}{\rho} \sqrt{-\rho^4 + \rho^2(\epsilon + 1) - j^2} = \frac{\hbar R_0^2}{2}\left(\frac{\epsilon + 1}{2} - j\right) \tag{4.34}$$

where $\rho_>$, $\rho_<$ are given by the two roots (4.11). Quantizing according to eqs. (4.2), (4.3) and solving for the energy levels we obtain

$$E_{n_r \ell} = \hbar \omega_0 (2n_r + \ell + 3/2) - \mu \tag{4.35}$$

i.e. the result which is obtained for the free trap, shifted by the change of the ground state energy due to the condensate.

Type B motion:

For this type of motion we have $j^2 < \epsilon$. The radial action is given by the integral

$$I_r(\epsilon, j) = \frac{\hbar R_0^2}{\pi} \int_{\rho_<}^{\rho_>} d\rho \left(\left(\epsilon^2 + (1 - \rho^2)^2 \Theta(1 - \rho)\right)^{1/2} - \frac{j^2}{\rho^2} - |1 - \rho^2|\right)^{1/2} \tag{4.36}$$

where $\rho_<$, $\rho_>$ are given by eqs. (4.8) and (4.15), respectively.

The integral can be performed in terms of elementary functions. We give a summary of the necessary steps in the appendix. The result is most succinctly expressed in terms of the functions

$$\int_A^{\pi/2} \frac{\cos^2 \varphi}{a + b \sin \varphi} d\varphi = \begin{cases} J_>(A, a, b) & a^2 > b^2 \\ J_<(A, a, b) & a^2 < b^2 \end{cases} \tag{4.37}$$

$$\int_A^{\pi/2} \frac{\cos^2 \varphi}{(a + b \sin \varphi)^2} d\varphi = \begin{cases} K_>(A, a, b) & a^2 > b^2 \\ K_<(A, a, b) & a^2 < b^2 \end{cases} \tag{4.38}$$

which can be written and programmed explicitly in terms of elementary functions. The radial action is then obtained in the form

$$I_r(\epsilon, j) = \frac{\hbar R_0^2}{\pi} \left\{ \sum_{i=1}^{3} C_i J_>(A_1, a_i, b_1) + C_4 J_<(A_1, a_4, b_1) \right.$$
$$\left. + C_5 K_<(A_1, a_4, b_1) + C_6 J_>(A_2, a_5, b_2) \right\} \tag{4.39}$$

with the parameters

$$A_1 = \arcsin\left(\frac{\epsilon^2 + j^2}{\epsilon\sqrt{1 + \epsilon^2 + 2j^2}}\right) \tag{4.40}$$

$$A_2 = \arcsin\left(\frac{1 - \epsilon}{\sqrt{(\epsilon + 1)^2 - 4j^2}}\right) \tag{4.41}$$

$$b_1 = \epsilon\sqrt{1 + \epsilon^2 + 2j^2} \tag{4.42}$$

$$b_2 = \sqrt{\left(\frac{\epsilon + 1}{2}\right)^2 - j^2} \tag{4.43}$$

$$a_{1,2} = \mp(\epsilon + j^2)\sqrt{\epsilon^2 + 1} + j^2(\epsilon - 1) \tag{4.44}$$

$$a_3 = -\epsilon - \epsilon^2 - 2j^2 \tag{4.45}$$

$$a_4 = \epsilon - \epsilon^2 \tag{4.46}$$

$$a_5 = \frac{\epsilon + 1}{2} \tag{4.47}$$

and the coefficients

$$C_{1,2} = \frac{1}{4} \left(1 - \epsilon \mp \sqrt{\epsilon^2 + 1} \right) \frac{\epsilon(1 + \epsilon^2 + 2j^2)}{\sqrt{\epsilon + j^2}} \tag{4.48}$$

$$C_3 = \frac{1}{4} \frac{\epsilon^2(1 + \epsilon^2 + 2j^2)}{\sqrt{\epsilon + j^2}} \tag{4.49}$$

$$C_4 = \frac{1}{4}(\epsilon - 2) \frac{\epsilon(1 + \epsilon^2 + 2j^2)}{\sqrt{\epsilon + j^2}} \tag{4.50}$$

$$C_5 = \frac{1}{2} \sqrt{\epsilon + j^2} \epsilon^2 (1 + \epsilon^2 + 2j^2) \tag{4.51}$$

$$C_6 = \frac{1}{8}(\epsilon + 1)^2 - \frac{1}{2}j^2 \,. \tag{4.52}$$

The semiclassical approximations for the quasi-particle excitation energies are now obtained by solving the equation

$$I_r \left(\frac{2E}{\hbar\omega_0 R_0^2}, \frac{\ell + 1/2}{R_0^2} \right) = \hbar(n_r + 1/2) \,. \tag{4.53}$$

for E. This last step cannot be done analytically, but it is easily accomplished numerically.

V. SEMICLASSICAL WAVE FUNCTIONS

For purely radial dynamics eq. (3.16) reduces to

$$\frac{1}{r^2} \frac{d}{dr} \left[a_0^2(r) r^2 \left(1 + \left(\sqrt{1 + E^2/K^2} - E/K \right)^2 \right) p_r \right] = 0 \tag{5.1}$$

which is easily solved, putting $[\ldots] = \text{const}$ in eq. (5.1). Inserting the result in eq. (3.13) we obtain the prefactors of the semiclassical wave function to lowest order. The exponential factors $\exp(\pm iS/\hbar)$ in (3.1) are combined to satisfy the usual matching conditions on the lower turning point. After some rearrangement in the prefactors we obtain

$$\begin{pmatrix} u_{n_r lm}(\boldsymbol{r}) \\ v_{n_r lm}(\boldsymbol{r}) \end{pmatrix} = \frac{C_0}{2r} \left(\frac{\sqrt{\sqrt{E^2 + K^2} + K} + \sqrt{\sqrt{E^2 + K^2} - K}}{\sqrt{\sqrt{E^2 + K^2} + K} - \sqrt{\sqrt{E^2 + K^2} - K}} \right) \cdot$$

$$\frac{\sin \left(\frac{1}{\hbar} \int_{r_<}^r p_r(r) dr + \frac{\pi}{4} \right)}{\sqrt[4]{E^2 + K^2} \sqrt{|p_r(r)|}} Y_{\ell m}(\vartheta, \varphi) \tag{5.2}$$

where $p_r(r)$, $K^2(r)$, are defined in eqs. (4.1), (4.4), and $r_< = \rho_< d_0 R_0$ given by eq. (4.8) for type B motion or (4.11) for type A motion. The normalization condition (2.13) serves to determine the constant C_0 by the integral

$$1 = \frac{C_0^2}{2} \int_{r_<}^{r_>} dr \frac{E}{\sqrt{E^2 + K^2}} \frac{1}{|p_r(r)|} = \frac{C_0^2}{4m} T_r \tag{5.3}$$

where T_r is the period of the radial motion, and $r_> = \rho_> d_0 R_0$ is defined by eq. (4.15). To obtain eq. (5.3) we have restricted the normalization integral to the classically allowed domain and replaced the rapidly oscillating $\sin^2(\hbar^{-1} \int^r p_r dr + \pi/4)$ by its average $1/2$. Furthermore we used the identities (3.18) for the radial velocity.

A. General case

The integral in eq. (5.3) can be carried out explicitly. The necessary steps are summarized in Appendix B. We obtain

$$C_0^2 = \begin{cases} \frac{4m\omega_0}{\pi} & \text{type A motion} \\ \frac{4m\omega_0}{\frac{\pi}{2} - \alpha + 4\epsilon\beta(2\epsilon^2 + 4j^2)^{-1/2}} & \text{type B motion} \end{cases} \tag{5.4}$$

with

$$\alpha = \arctan \frac{1-\epsilon}{2\sqrt{\epsilon - j^2}}$$

$$\beta = \arctan \left[\frac{\sqrt{\epsilon - j^2}}{\sqrt{2(\epsilon^2 + 2j^2)}} \frac{\epsilon + \epsilon^2 + 2j^2 + \epsilon\sqrt{1+\epsilon^2+2j^2}}{\epsilon^2 + j^2 + \epsilon\sqrt{1+\epsilon^2+2j^2}} \right]. \tag{5.5}$$

Using these results it can be shown that for type B-motion the wave-functions for large energy tend to those of the free harmonic trap.

B. Large condensate

The result (5.4) simplifies if we consider the limit $R_0 \to \infty$, keeping

$$E = \frac{1}{2}\hbar\omega_0 R_0^2 \epsilon, \quad \ell + 1/2 = R_0^2 j \tag{5.6}$$

fixed. Type A motion disappears in that limit and for type B motion we obtain

$$C_0^2 = \frac{2m\omega_0}{\pi}\sqrt{2 + \hbar^2\omega_0^2(\ell + 1/2)^2/E^2}. \tag{5.7}$$

The correctly normalized wave functions (5.2) can now be used to evaluate matrix elements in the semiclassical limit. This will be done in the next section to calculate the cross section for inelastic light scattering by which a quasi-particle is created from the condensate.

VI. SEMICLASSICAL STRUCTURE FUNCTION

To introduce the dynamical structure function let us first consider the differential cross-section for the off-resonant scattering of light from the trapped gas. Light with incoming wave-vector and frequency $\boldsymbol{q}_L, \omega_L$ is scattered into an outgoing field with $\boldsymbol{q}'_L = \boldsymbol{q}_L - \boldsymbol{k}, \omega'_L = \omega_L - \omega$ with $\omega \ll \omega_L$. The scattering angle θ between $\boldsymbol{q}'_L$ and $\boldsymbol{q}_L$ is related to k by the usual kinematical relation $ck = 2\omega_L sin(\theta/2)$ which implies the allowed interval $0 < k < 2\omega_L/c$. The permitted interval for the transferred frequency ω can be estimated from the corresponding relation for free atoms $0 < \omega < (2\hbar\omega_L^2/mc^2)$. Let now the differential cross-section for the off-resonant light scattering from a single atom in its ground state be given by $(d\sigma/d\Omega)_{At}$. Then the spectral distribution of the differential cross-section for light scattering off the trapped atomic gas is given by [18,19]

$$\frac{d\sigma}{d\Omega d(\hbar\omega)} = \left(\frac{d\sigma}{d\Omega}\right)_{At} S(\boldsymbol{k}, \omega). \tag{6.1}$$

The dynamical structure function $S(\boldsymbol{k}, \omega)$ is the Fourier transform of the density — density correlation function and defined as the thermal expectation value

$$S(\boldsymbol{k}, \omega) = \frac{1}{Z} \sum_{\mu,\mu'} e^{-\beta E_\mu} |\langle \mu'|\rho(\boldsymbol{k})|\mu\rangle|^2 \delta(\hbar\omega + E_\mu - E_{\mu'}). \tag{6.2}$$

Here $|\mu\rangle$ and E_μ are energy eigenstates and levels of the system, and

$$\rho(\boldsymbol{k}) = \int d^3r \, \psi^+(\boldsymbol{r}) e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} \psi(\boldsymbol{r}) \tag{6.3}$$

is the operator of the density fluctuation with wave vector $\boldsymbol{k}$.

In the present case $S(\boldsymbol{k}, \omega)$ assumes the form

$$S(\boldsymbol{k}, \omega) = S_0(\boldsymbol{k})\delta(\hbar\omega) + {\sum_i}' S_i(\boldsymbol{k}) \left[\delta(\hbar\omega + E_i) + e^{-\beta E_i}\delta(\hbar\omega - E_i) \right]$$

$$+ {\sum_{ij}}' S_{ij}^{(1)}(\boldsymbol{k}) \left[\delta(\hbar\omega + E_i + E_j) + e^{-\beta(E_i+E_j)}\delta(\hbar\omega - E_i - E_j) \right]$$

$$+ {\sum_{ij}}' S_{ij}^{(2)}(\boldsymbol{k})\Theta(E_i - E_j) \left[\delta(\hbar\omega + E_i - E_j) + e^{-\beta(E_i-E_j)}\delta(\hbar\omega - E_i + E_j) \right], \tag{6.4}$$

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where the sums $\sum'$ run over the quasi-particle states with $E_i \neq 0$. The first term in eq. (6.4) describes coherent elastic scattering, and $S_0(\boldsymbol{k})$ is simply the square of the Fourier transform of the density

$$S_0(\boldsymbol{k}) = \left| \int d^3 r e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} \left\{ |\psi_0(\boldsymbol{r})|^2 + {\sum_i}' |v_i(\boldsymbol{r})|^2 + {\sum_i}' \left(|u_i|^2 + |v_i|^2 \right) \left(e^{\beta\hbar\omega_i} - 1 \right)^{-1} \right\} \right|^2 . \tag{6.5}$$

Because $\psi_0 \propto \sqrt{N_0}$ this is by far the dominant contribution in $S(\boldsymbol{k}, \omega)$. This contribution of the scattered light, by its interference with the non-scattered light, is used in the phase-contrast imaging of the condensates [27]. The part $\sum_i' |v_i(\boldsymbol{r})|^2$ gives the number density of particles outside the condensate at temperature $T = 0$ due to the interaction. It can be easily seen from eq. (5.2) that $|v_i(\boldsymbol{r})|^2$ vanishes for $r > r_0$. For weak interaction this number density is much smaller than N_0/r_0^3.

The second term in eq. (6.4) describes the creation of a quasi-particle from the condensate. The matrix element for this process is

$$M_i^*(\boldsymbol{k}) = \int d^3 r \, e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \psi_0(\boldsymbol{r})(u_i^*(\boldsymbol{r}) - v_i^*(\boldsymbol{r})) \tag{6.6}$$

and

$$S_i(\boldsymbol{k}) = |M_i(\boldsymbol{k})|^2 (\bar{n}_i + 1), \quad \bar{n}_i = \frac{1}{e^{\beta E_i} - 1} \tag{6.7}$$

The other quantities in (6.4) are:

$$M_{ij}^{(1)*}(\boldsymbol{k}) = -\int d^3 r \, u_i^* v_j^* e^{i\boldsymbol{k}\cdot\boldsymbol{r}}, \quad M_{ij}^{(2)*}(\boldsymbol{k}) = \int d^3 r \, (u_i^* u_j + v_i^* v_j) e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$$

$$S_{ij}^{(1)}(\boldsymbol{k}) = \left| M_{ij}^{(1)}(\boldsymbol{k}) \right|^2 \sqrt{(\bar{n}_i + 1)(\bar{n}_j + 1)}, \quad S_{ij}^{(2)}(\boldsymbol{k}) = \left| M_{ij}^{(2)}(\boldsymbol{k}) \right|^2 \sqrt{(\bar{n}_i + 1)\bar{n}_j} \tag{6.8}$$

Here $S_{ij}^{(1)}$ is proportional to the cross-section for the absorption of an energy $\hbar\omega$ by creating a pair of quasi-particles with energies E_i, E_j from the condensate. The cross-section for the time-reversed process is smaller by a factor $e^{-\beta(E_i+E_j)}$ due to detailed balance. Similarly $S_{ij}^{(2)}\Theta(E_i - E_j)$ describes the cross-section for absorbing an energy $\hbar\omega$ by converting a quasi-particle of energy E_j into one with energy E_i. Both $S_{ij}^{(1)}$ and $S_{ij}^{(2)}$ give rise to a faint and broad spectral background in the scattering. In the following we shall therefore content ourselves with the evaluation of $|M_i(\mathbf{k})|^2$.

A. General case

Here we shall evaluate the matrix element (6.6) in the semiclassical limit. It is clear that only type B motion can contribute, because otherwise ψ_0 and $(u_i - v_i)$ don't overlap. The condensate wave function is given by eq. (2.5). The amplitude $(u_i - v_i)$ is obtained from eq. (5.2), and $e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}$, where $\boldsymbol{k}$ in z-direction in semiclassical approximation is expanded as

$$e^{-ikz} = \sum_{\ell=0}^{\infty} (-i)^\ell \frac{2}{r} \sqrt{\frac{\pi(2\ell+1)}{k}} \frac{1}{\sqrt[4]{k^2 - \left(\frac{\ell+1/2}{r}\right)^2}}$$

$$\cos\left(\int_{\left(\frac{\ell+1/2}{k}\right)}^{r} \sqrt{k^2 - \left(\frac{\ell+1/2}{r}\right)^2} - \frac{\pi}{4} \right) Y_{\ell 0}(\Theta, \Phi) . \tag{6.9}$$

The integral (6.6) is to be taken over the angles Θ, Φ selecting the angular momentum quantum number from the sum in (6.5) and over $r^2 dr$ from $r = r_<$ to $r = r_0$. This radial integral is of the general form

$$\int_{r_<}^{r_0} dr \, f(r) \cos \varphi(r) \simeq \sqrt{\frac{2\pi}{|\varphi''(z_0)|}} f(z_0) \cos\left(\varphi(z_0) + \operatorname{sgn}\left(\varphi''(z_0)\right) \frac{\pi}{4} \right) \tag{6.10}$$

where the evaluation is done in the stationary phase approximation and z_0 is defined as solution of $\varphi'(z_0) = 0$ in the interval $r_< < z_0 < r_0$. Before writing the integral explicitly we introduce scaled parameters and variables as before and in addition

$$k = R_0 \kappa / d_0 \quad , \quad C_0 = \sqrt{m \omega_0 \tilde{C}} . \tag{6.11}$$

Then, neglecting a rapidly oscillating term without stationary phase in the interval $r_< < r < r_0$, the amplitude can be written as

$$M_{n_r l m}(k) = \delta_{m0}(-i)^\ell \sqrt{\frac{\tilde{C}}{\kappa}} \frac{1}{R_0^2} \sqrt{\frac{15 N_0 (2\ell + 1)}{8}} \int_{\max(j/\kappa, \rho_<)}^1 d\rho \sqrt{1 + \frac{1 - \rho^2}{\sqrt{\epsilon^2 + (1 - \rho^2)^2}}}$$

$$\frac{\sqrt{1 - \rho^2}}{\sqrt{\pi_w(\rho)}} \cdot \frac{1}{\sqrt{\pi_r(\rho)}} \cos \left[R_0^2 \int_{\rho_<}^\rho d\rho' \pi_r(\rho') - R_0^2 \int_{j/\kappa}^\rho d\rho' \pi_w(\rho') \right] . \tag{6.12}$$

with $\pi_r(\rho)$ given by eq. (4.7) and

$$\pi_w(\rho) = \sqrt{\kappa^2 - j^2/\rho^2} \tag{6.13}$$

The stationary point z_0 is determined by

$$\pi_r(z_0) = \pi_w(z_0) \tag{6.14}$$

which is solved by

$$z_0 = \sqrt{\frac{\kappa^4 + 2\kappa^2 - \epsilon^2}{2\kappa^2}} . \tag{6.15}$$

Now we have to examine under which conditions z_0 lies in the required interval:
i) The condition for ψ_0, $u - v$, and e^{-ikz} to overlap are

$$\epsilon > j^2 \quad , \quad j < \kappa \tag{6.16}$$

ii) z_0 satisfies $0 \leq z_0^2 \leq 1$ if

$$\kappa^4 + 2\kappa^2 \geq \epsilon^2 \geq \kappa^4 \tag{6.17}$$

iii) z_0 satisfies the lower bound $j/\kappa \leq z_0$ if

$$\epsilon^2 \leq \kappa^4 + 2\kappa^2 - 2j^2 \tag{6.18}$$

which is stronger than the first inequality (6.17) if the second inequality (6.17) holds.
iv) z_0 satisfies the lower bound $\rho_< \leq z_0$ if

$$\sqrt{1 + \epsilon^2 + 2j^2} \leq 1 + \frac{\epsilon^2(\kappa^4 + 2\kappa^2 - 2j^2 - \epsilon^2) + 2j^2\kappa^4}{2j^2\kappa^2} . \tag{6.19}$$

It follows from (6.18) that the right hand side of (6.19) is positive. Therefore both sides of (6.19) can be squared without changing the inequality, and we obtain after some rearrangements instead of (6.19)

$$\left[j^2 + \left(\frac{\epsilon^2 - \kappa^4}{2\kappa^2} \right) \left(1 - \frac{\epsilon^2 - \kappa^4}{2\kappa^2} \right) \right]^2 \leq \left[\left(1 - \frac{\epsilon^2 - \kappa^4}{2\kappa^2} \right) \left(\frac{\epsilon^2 + \kappa^4}{2\kappa^2} \right) \right]^2 . \tag{6.20}$$

The terms inside the brackets [...] on both sides of (6.20) are positive, by virtue of eq. (6.17). Therefore we may take the square root of both sides of eq. (6.20), to obtain after some more rearrangements, again the inequality (6.18). Thus, eq. (6.19) leads to no additional condition if inequalities (6.16)–(6.18) are satisfied, which are therefore the semiclassical selection rules for the creation of quasi-particles from the condensate. For later reference it is usefull to rewrite the most restrictive of these inequalities in dimensional quantities as follows

$$\frac{\hbar^2 k^2}{2m} \leq E_{n_r \ell} \leq \sqrt{\left(\frac{\hbar^2 k^2}{2m}\right)^2 + \mu \frac{\hbar^2 k^2}{m} - \frac{1}{2}(\ell + \frac{1}{2})^2(\hbar\omega_0)^2} \,. \tag{6.21}$$

A numerical example for this selsction rule is shown in Fig. 5.

Next we need to determine $\pi_w(z_0) = \pi_r(z_0)$ and obtain

$$\pi_w(z_0) = \kappa \sqrt{\frac{\kappa^4 + 2\kappa^2 - \epsilon^2 - 2j^2}{\kappa^4 + 2\kappa^2 - \epsilon^2}} \,. \tag{6.22}$$

We also need the sign of

$$\varphi''(z_0) = R_0^2(\pi_r'(z_0) - \pi_w'(z_0)) = R_0^2 \frac{2\kappa^2}{\epsilon^2 + \kappa^4} \frac{\kappa^4 + 2\kappa^2 - \epsilon^2}{\sqrt{2(\kappa^4 + 2\kappa^2 - \epsilon^2 - 2j^2)}} \tag{6.23}$$

which is evaluated to be positive. We can now apply the formula (6.9) to (6.11) and obtain

$$M_{n_r lm}(k) = (-i)^\ell \delta_{m0} \sqrt{\frac{\tilde{C}}{\kappa}} \frac{\epsilon}{\kappa^3 R_0^3} \sqrt{\frac{15\pi N_0(2\ell + 1)\sqrt{2}}{8}} \frac{\sqrt{\epsilon^2 - \kappa^4}}{\sqrt[4]{\kappa^4 + 2\kappa^2 - \epsilon^2 - 2j^2}} \cos\left(\varphi + \frac{\pi}{4}\right) \tag{6.24}$$

where the phase φ

$$\varphi = \varphi_1 + \varphi_2 \tag{6.25}$$

is given by the integrals

$$\varphi_1 = R_0^2 \int_{\rho_<}^{z_0} d\rho \pi_r(\rho)$$

$$\varphi_2 = -R_0^2 \int_{j/\kappa}^{z_0} d\rho \pi_w(\rho) \,. \tag{6.26}$$

Integrals of this kind had already to be evaluated when calculating the action I_r, and the same substitutions as were made there are also of help here. In fact the integrals (6.26) and (4.36) differ only by a prefactor $\hbar/\pi$ and by the upper boundary. Using this observation we obtain by the series of steps summarized for eq. (4.36) in appendix A a result for (6.26) which differs from (A5) only by the prefactor and the boundary $A_1 \rightarrow A_3$ with

$$A_3 = \arcsin\left[\frac{\epsilon - \kappa^2 + \epsilon^2 + \epsilon\kappa^2 + 2j^2}{(\epsilon + \kappa^2)\sqrt{1 + \epsilon^2 + 2j^2}}\right] \,. \tag{6.27}$$

Explicitely

$$\varphi_1 = R_0^2 \left\{ \sum_{i=1}^3 C_i J_>(A_3, a_i, b_1) + C_4 J_<(A_3, a_4, b_1) + C_5 K_<(A_3, a_4, b_1) \right\} \tag{6.28}$$

with the parameters given by eqs. (4.42)–(4.51). The second integral (6.26) is simplified by the substitution

$$\rho = \frac{j}{\kappa \cos u} \tag{6.29}$$

and gives, after evaluation

$$\varphi_2 = -R_0^2 j \left\{ \sqrt{\frac{\kappa^4 + 2\kappa^2 - \epsilon^2}{2j^2} - 1} - \arccos\left(\frac{\sqrt{2}j}{\sqrt{\kappa^4 + 2\kappa^2 - \epsilon^2}}\right) \right\} \,. \tag{6.30}$$

Now the matrix element is completely determined in the semiclassical approximation. The inelastic part of the structure function (6.4) at $T = 0$ can be given by the sum

$$S^{(1)}(\boldsymbol{k},\omega) = \frac{\pi d_0 \omega^2}{\sqrt{2}a(kd_0)^7\hbar\omega_0^3} {\sum_{n_r}}' {\sum_\ell}' \frac{\tilde{C}_{n_r\ell}(2\ell+1)\left[(2\omega/\omega_0)^2 - (kd_0)^4\right]}{\sqrt{(kd_0)^4 + 2(kd_0)^2 R_0^2 - (2\omega/\omega_0)^2 - 2\left(\ell + \frac{1}{2}\right)^2}}$$

$$\cdot \left(\frac{1 - \sin 2\varphi_{n_r\ell}}{2}\right)\delta\left(\frac{\omega + \omega_{n_r l}}{\omega_0}\right) \tag{6.31}$$

where the two sums are restricted to quantum numbers n_r, ℓ satisfying the semiclassical selection rules (6.16)–(6.18) with $\epsilon = \hbar\omega_{n_r\ell}/\mu$ and $j = (\ell + \frac{1}{2})/R_0^2$. Here we have put indices n_r, ℓ on $\tilde{C}$ and φ defined by eqs.(6.11),(5.4) and (6.25), respectively, to indicate the dependence of these quantities on the quantum numbers n_r,ℓ via $\epsilon = \hbar\omega_{n_r\ell}/\mu$ and $j = (\ell + \frac{1}{2})/R_0^2$.

B. Limit of large condensate

In the limit of a large condensate $R_0 >> 1$, $E/\hbar\omega_0 \sim 0(1)$, $(\ell + 1/2) \sim 0(1)$, $kR_0d_0 \sim 0(1)$ the result (6.31) for the inelastic structure function simplifies. For the prefactor $\tilde{C}_{n_r\ell}$ we can use the asymptotic form (5.7) with eq. (6.11). The semiclassical selection rules (6.16)–(6.18) take the form

$$E_{n_r\ell} \geq \frac{1}{2}\hbar\omega_0\frac{(\ell + 1/2)^2}{R_0^2} \quad ; \quad \ell + 1/2 \leq R_0 kd_0 \tag{6.32}$$

$$\frac{1}{2}\hbar\omega_0(kd_0)^2 \leq E_{n_r\ell} \leq \frac{1}{\sqrt{2}}\hbar\omega_0\sqrt{R_0^2(kd_0)^2 - (\ell + 1/2)^2} \tag{6.33}$$

where the right-hand side of (6.33) has been simplified using $(kd_0/R_0)^2 << 1$.

The first condition of (6.32) is always satisfied for sufficiently large R_0, the second represents a restriction on the size of ℓ since we want to assume $R_0 kd_0 \sim 0(1)$. In (6.33) we can use the result (4.25) for the quasi-particle energies in large condensates and obtain

$$2n_r + \ell + 3/2 \leq R_0 kd_0 \tag{6.34}$$

for the second inequality in (6.33), while the first is always satisfied in the limit we consider. It is somewhat surprising to see the energy levels of the free trap appearing in (6.34). Under the square-root in the denominator of eq. (6.31) and also in the nominator we may again neglect $(kd_0)^4$ compared to the other terms. Finally, the tedious general results (6.28), (6.30) with (4.40)–(4.51) for φ_1 and φ_2 may be simplified considerably by using the asymptotic results (4.18), (4.19) for $\rho_<$ and π_r, and

$$z_0 \to \sqrt{1 - 2(\omega_{n,\ell}/\omega_0 R_0 kd_0)^2} \tag{6.35}$$

$$\pi_w(\rho) = \frac{1}{R_0^2}\sqrt{(R_0 kd_0)^2 - (\ell + 1/2)^2/\rho^2} \tag{6.36}$$

following from eqs. (6.15), (6.13) in eqs. (6.26). The integrals are now much easier to perform and we obtain after some further rearrangements

$$\varphi_{n_r\ell}(k) = -R_0 kd_0\left(\sin\chi_{n_r\ell}(k) - \chi_{n_r\ell}(k)\cos\chi_{n_r\ell}(k)\right) \tag{6.37}$$

with the angle $\chi_{n_r\ell}(k)$ defined by

$$\cos\chi_{n_r\ell}(k) = \frac{2n_r + \ell + 3/2}{R_0 kd_0}. \tag{6.38}$$

The inequality (6.34) is incorporated in this definition. After all this the structure function (6.31), in the limit of large condensates, takes the explicit form

$$S^{(1)}(\boldsymbol{k},\omega) = \frac{d_0}{a\hbar\omega_0}\frac{4}{(kd_0)^7}\left|\frac{\omega}{\omega_0}\right|^3 \sum_{\substack{n_r \\ (2n_r+\ell+3/2\leq R_0 kd_0)}}\sum_\ell \frac{(2n_r + \ell + 3/2)(2\ell+1)}{\sqrt{(R_0 kd_0)^2 - (2n_r + \ell + 3/2)^2}}$$

$$\cos^2\left(\frac{\pi}{4} + \varphi_{n_r\ell}(k)\right)\delta\left((\omega + \omega_{n_r\ell})/\omega_0\right) \tag{6.39}$$

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with $\varphi_{n_r\ell}$ and $\omega_{n_r\ell}$ given by eqs. (6.37) and (4.25) respectively. It is interesting to note that $S^{(1)}(\mathbf{k},\omega)$ in the present limit has resonances for the *maximum* momentum transfer $R_0 k d_0 = 2n_r + \ell + 3/2$ by which states with the principal quantum number $n = 2n_r + \ell$ can be excited. The angles $\chi_{n_r\ell}(k)$ and $\varphi_{n_r\ell}(k)$ vanish there. Similar resonances appear also in the more general result (6.31) which diverges whenever the border of the semiclassical selection rule (6.18) is approached.

VII. SOME NUMERICAL EXAMPLES

All the calculations, so far, have been analytical, but the final results for the energy levels, wave functions and inelastic structure function are not obtained in explicit form and must be evaluated numerically from the implicit results we have derived. This can be done without difficulty. We shall here consider some examples of such results:

A. Energy levels:

The energy levels are obtained by solving eq. (4.53) for E. This can be done numerically without difficulty and ambiguity, since

$$\frac{\partial I_r}{\partial E} = \frac{T_r}{2\pi} > 0 \tag{7.1}$$

where T_r is the period of the radial motion. In Fig. 2 we take $(\mu/\hbar\omega_0) = \frac{1}{2}R_0^2 = 4.27$ and plot the level shifts $\delta_n(\ell)$ defined as a function of ℓ and the *principal* quantum number $n = \ell + 2n_r$ by

$$\hbar\omega_0 \delta_n(\ell) = E_{n_r\ell} + \mu - \hbar\omega_0(n + 3/2). \tag{7.2}$$

As for type A motion the levels are the same as for the free trap, apart from a shift in the zero-point energy from $3\hbar\omega_0/2$ to $3\hbar\omega_0/2 - \mu$, it is clear that (7.2) vanishes for this type of motion, characterized by the simultaneous inequalities $1 \leq 2j - 1 \leq \epsilon \leq j^2$, which imply

$$(E_{n_r\ell} + \mu)/\hbar\omega_0 \geq (\ell + 1/2) \geq (2E_{n_r\ell}/\hbar\omega_0)^{1/2}(2\mu/\hbar\omega_0)^{1/2}. \tag{7.3}$$

The first inequality must always be satisfied for energy levels to exist, at least semiclassically, i.e. there are no levels where it is violated (cf. eq. (4.12)). The second inequality marks the border in the (n,ℓ)-plane in Fig. 2 where $\delta_n(\ell)$ drops to 0. For type B motion $\ell_r + 1/2 \leq (2E_{n_r\ell}/\hbar\omega_0)^{1/2}(2\mu/\hbar\omega_0)^{1/2}$ is satisfied. The level shifts are positive due to the repulsion provided by the condensate. This repulsion is stronger for the lower lying levels, as one could expect.

B. Structure function:

The dynamical structure function in the approximation we have considered is determined, up to prefactors, by just two parameters, R_0^2 which fixes the number of particles of a given atomic species in a given trap via $N_0 = \sqrt{\hbar/m\omega_0}R_0^5/15a$, and kd_0 which fixes the scattering angle via $\theta = 2 Arcsin\left[kd_0(\lambda/4\pi)(m\omega_0/\hbar)^{1/2}\right]$, where λ is the wavelength of the scattered light. We shall assume that the wavelength of the light used in the scattering experiment is off-resonance but roughly given by the D-line of the alkali-metal, i.e. $\lambda \approx 590$ nm for sodium, and $\lambda \approx 800$ nm for rubidium.

The result (6.31) for the inelastic part of the structure function for $R_0^2/2 = \mu/\hbar\omega_0 = 4.27$ and $kd_0 = 15.1$ is plotted in Fig. 3. For a trap with frequency $\nu_0 = \omega_0/2\pi = 100$ Hz these numbers correspond to light scattering from a ^{23}Na condensate of $N_0 \approx 8000$ atoms with $\theta \approx 40^o$ or from a ^{87}Rb condensate of $N_0 \approx 4000$ atoms with $\theta \approx 126^o$. This is a typical example for light scattering with a large momentum transfer in which high-lying quasi-particle states are excited. The plot gives as discrete points the strength of the δ-functions in eq. (6.31), which according to our sign convention for ω appear at negative values $\omega = -E_{n_r\ell}/\hbar$ for absorption of energy. Since we consider temperature $T = 0$ in the plots of Figs. 3, 4, 6 the emission lines at positive $\omega = E_{n_r\ell}/\hbar$ are frozen out. The infinitely sharp lines described by the δ-functions are, of course, not directly observable. Apart from the intrinsic line-widths which we did not consider in this work, they must also be convoluted with the experimental resolution. However, in order to retain the full information present in eq. (6.31), we prefer not to carry out such an arbitrary smoothing. The inelastic part of the structure function is seen to consist of several discrete quasi-continuous rotational bands, roughly spaced

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by $\hbar\omega_0$. In the region of parameter space chosen here, these bands can be usefully labelled by the principal quantum number $n = 2n_r + \ell$ of the free trap, in terms of which the energy levels are expressed as

$$E_{n_r\ell} = \hbar\omega_0(n + 3/2) - \mu + \hbar\omega_0\delta_n(\ell). \tag{7.4}$$

If $\delta_n(\ell) = 0$ were satisfied each band would collapse to a single sharp line. The semiclassical selection rule (6.17) limits the excited bands to the domain

$$\frac{1}{2}\sqrt{(kd_0)^4 + 2R_0^2(kd_0)^2} \geq \frac{E_{n_r\ell}}{\hbar\omega_0} \geq \frac{(kd_0)^2}{2}. \tag{7.5}$$

In the present case $(kd_0)^2 >> 2R_0^2$ we may simplify this relation somewhat by expanding the square root and using $R_0^2 = 2\mu/\hbar\omega_0$ to obtain an energy interval of size μ for the excited quasi-particle states which extends above the recoil energy $\hbar^2 k^2/2m$

$$\frac{(kd_0)^2}{2} + \frac{\mu}{\hbar\omega_0} \geq \frac{E_{n_r\ell}}{\hbar\omega_0} \geq \frac{(kd_0)^2}{2}. \tag{7.6}$$

In the local density approximation [22] the structure function is just a single continuous band in the same energy interval (and a corresponding band at negative energies related by detailed balance). It is not surprising that our treatment, being based on the discrete quasi-particle states, reveals considerably more structure, namely the bands and their discrete substructure. As can be seen from (7.6) the number of bands in Fig. 3 just gives the integer part of $\mu/\hbar\omega_0$. This rather direct physical measure of μ in units of $\hbar\omega_0$ could be of practical experimental interest. The fine structure of the rotational bands is also determined by the semiclassical selection rules (6.16)–(6.18). The rotational quantum number ℓ increases within each band of Fig. 3 from left to right. The strongest line within each band corresponds to the maximum value $\ell_{max}(n)$ of ℓ permitted by eq. (6.18) for type B motion.

We can compare these results with similar ones one may infer from Fig. 2 of ref. [14], where the quasi-continuous rotational bands due to high-lying quasi-particle states were first found. The results in [14] were obtained by a much simpler approximation, not aiming at achieving full self-consistency, using the excited state wave functions of the empty trap, rather than the WKB wave functions whose use underlies the present Fig. 3. This implies that $\pi_r(\rho)$ in eq. (6.12) is replaced by the free oscillator expression

$$\pi_r^0 = \sqrt{\epsilon - j^2/\rho^2 - \rho^2}. \tag{7.7}$$

Of course this leads to much simpler closed formulas for $|M_{n,\ell}(k)|^2$ (eqs. (5), (6) of ref. [14]). However, with our present self-consistent treatment we are now able to assess the limitations of the simpler approximation. In fact, the result presented in Fig. 3 differs in two important details from that of [14]:
(i) There is an overall shift of size μ of the energy window excited by the transferred wave number k, and (ii) there is a qualitative change in the dependence of the width of the rotational bands on the principal quantum number which, according to Fig. 3, become more narrow as the principal quantum number increases, while the opposite behavior was found in [14]. Both differences have their origin in a change in the semiclassical selection rules (6.16)–(6.18), which depend rather sensitively on approximations in the phases of the wave functions inside the condensate. The first shortcoming of the approximation in [14] can be easily eliminated by using simply $E_n^{osc} = \hbar\omega_0(n + 3/2) - \mu$ rather than the free trap energies in the expressions for the free trap eigenfunctions. The second is not as easily avoided, however. It simply shows that the influence of the interaction with the condensate on the spatial dependence of the phase of the high lying states cannot be neglected as long as the widths Δ_n of the rotational bands given by $\Delta_n = \delta_n(0) - \delta_n(\ell_{max}(n))$ with

$$\ell_{\max}(n) + 1/2 = \sqrt{2}\left((kd_0)^4/4 + (kd_0)^2\mu/\hbar\omega_0 - (E_n^{osc}/\hbar\omega_0)^2\right)^{1/2} \tag{7.8}$$

are not themselves negligible. We conclude that for a proper treatment of the rotational bands the present treatment is indispensable.

The spectroscopic resolution of the quasi-continuous bands requires a resolution better than the widths Δ_n, which may be difficult to attain in the frequency domain, but could be feasible in real-time experiments extended over a time-scale of ≈ 10 periods $2\pi/\omega_0$. In real time the width Δ_n would turn up as collapse rate $\gamma_n = \Delta_n$ determining the dephasing of the band with principal quantum number n. Due to the discrete substructure of the bands this dephasing should in principle be reversible. However it appears unlikely that the strict phase coherence over a time-interval of the order of $\ell_{max}(n)/\Delta_n$, required to see such a rephasing, could be achieved experimentally. For a discussion of collapses and revivals of low-lying collective modes see [28] [29].

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Let us now look at the dynamical structure function also for smaller momentum transfer and for somewhat larger condensates. In fig. 4 we have chosen the parameters $R_0^2 = 11.24$, $kd_0 = 3$ corresponding to, $N_0 = 6000$, $\theta = 21°$ for ^{87}Rb and to $N_0 = 12000$, $\theta = 7.7°$ for ^{23}Na, if the same choices are made for ν_0 and λ as before. The changes in the scale in fig. 4 in comparison with fig. 3 should be noted. In fig. 4 we have joined spectral lines with equal principal quantum number $n = 2n_r + \ell$ by straight lines. This is usefull because the quantum number n organizes the spectral lines according to multiplets of different strengths. However, differently to the case of high lying states, where n labelled well-separated quasi-continuous bands, the different multiplets now overlap at least partially in their energy range. The strongest multiplet in fig. 4 corresponds to $n = 9$, the next to $n = 8$, and the third and weakest one shown to $n = 7$. There are actually still weaker lines with $n \leq 6$ which we have suppressed. All the lines satisfy the semiclassical selection rule (6.21). It is plotted for this case in fig. 5 in the (angular momentum, energy)-plane, together with the semiclassical energy levels. All levels within the curved triangular section of the plane satisfy the selection rule. In this plot multiplets of fixed $n = 2n_r + \ell$ lie on lines roughly parallel to the upper border of the triangular shape, the higher lying lines corresponding to higher values of n. On this upper border the square-root in the denominator of the expression (6.31) for $S^{(1)}(\mathbf{k}, \omega)$ vanishes, leading to a scattering singularity, while on the lower border the nominator of this expression vanishes, leading to a suppression of scattering. This observation explains qualitatively the dependence of the scattering cross-section on n. The multiplet with $n = 9$ consists only of the two lines for $\ell = 1$, $\ell = 3$. The remaining $\ell = 5$, $\ell = 7$, $\ell = 9$ members of this multiplet have smaller energy but lie above the triangular region in fig. 5. This highest lying multiplet of fig. 5 is therefore rather narrow and well separated in energy from the other multiplets. It lies entirely above the chemical potential μ, i.e. its lines in fig. 4 lie at $\omega/\omega_0 < \mu/\hbar\omega_0 = -5.62$. With these features this multiplet bears some resemblance to the well-separated bands of fig. 3. In contrast to this the two lower lying and weaker multiplets in fig. 4 overlap completely with each other and extend over energy levels ranging from values larger to values smaller than μ and already resemble the low lying multiplets extending down to the hydrodynamic regime. This can be seen from fig. 6 where we have chosen $R_0^2 = 26.2$, $kd_0 = 2$ corresponding to $N_0 = 50000$, $\theta = 14°$ for ^{87}Rb and $N_0 = 10^5$, $\theta = 5.2°$ for ^{23}Na, again assuming a trap of $\nu_0 = 100$ Hz and off-resonance scattering at wavelengths roughly equal to the respective D-lines. The multiplets are still organized according to their strengths by the principal quantum number n. However, now these multiplets are completely overlapping, much as the two lower lying ones in fig. 4. For the multiplets shown in fig. 6 n ranges from $n = 8$ for the strongest multiplet to $n = 6$ for the weakest one shown in the figure, but again we have suppressed in the plot still weaker lines corresponding to multiplets with smaller values of n. The dependence of the scattering cross-section on n, and within a given multiplet on ℓ, can be understood similarly to our discussion of fig. 4 by using the asymptotic expression (6.38) for $S^{(1)}(\mathbf{k}, \omega)$. Taken together the plots fig. 3–fig. 6 show that a measurement of $S(\mathbf{k}, \omega)$ over a range of scattering angles θ in principle can give a very detailed information on the quasiparticle levels in any energy interval selected by the choice of k according to eq. (6.21).

VIII. CONCLUSIONS

In the present paper we have solved the Bogoliubov equations for the elementary excitations of a Bose-condensed gas of atoms trapped in an isotropic harmonic potential in WKB-approximation. The underlying classical dynamics is integrable in this case due to the rotational symmetry. The quasi-particle energies in the trap have been obtained from a Bohr-Sommerfeld quantization rule. Corrections to that rule due to the non-differentiabilty of the condensate wave function in Thomas-Fermi approximation have been discussed in [15]. The mode-functions, including the Bogoliubov amplitudes v_j, have been obtained in the classically allowed regime in the WKB-form. Our results interpolate between the low-energy regime $E/\mu \to 0$, where asymptotically exact results within the Bogoliubov approximation are available [9] and the high-energy regime $\mu/E \to 0$, where perturbation theory can be used. As an application we have given a self-consistent calculation of the fully resolved dynamical structure function $S(k, \omega)$, which could be measured in off-resonant light scattering, in a large energy domain extending to all but the lowest lying levels.

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APPENDIX A: EVALUATION OF THE ACTION INTEGRAL

Here we summarize the essential steps for the evaluation of the integral in eq. (4.36). The integral is splitted into two parts, the first part $I_<$ taken over ρ from $\rho_<$ to 1, the second part $I_>$ taken over ρ from 1 to $\rho_>$. Let us consider the evaluation of $I_<$ first. The substitution

$$\rho = \sqrt{1 - \frac{2\epsilon t}{1 - t^2}}$$

$$d\rho = -\epsilon \frac{(1 + t^2)}{(1 - t^2)^{3/2}(1 - t^2 - 2\epsilon t)^{1/2}} dt \tag{A1}$$

transforms $I_<$ into an integral over t from

$$t = 0 \quad \text{to} \quad t = t_{\max} = \frac{-(\epsilon^2 + j^2) + \epsilon\sqrt{1 + \epsilon^2 + 2j^2}}{\epsilon + j^2} . \tag{A2}$$

A partial fraction expansion of the integrand results in the explicit form

$$I_< = \frac{\hbar R_0^2}{\pi} \epsilon \sqrt{\epsilon^2 + j^2} \int_0^{t_{\max}} dt \sqrt{\frac{\epsilon^2(1 + \epsilon^2 + 2j^2)}{(\epsilon + j^2)^2} - \left(t + \frac{\epsilon^2 + j^2}{\epsilon + j^2}\right)}$$

$$\left\{ \frac{\sqrt{\epsilon^2 + 1} + \epsilon - 1}{4\epsilon^2} \frac{1}{\sqrt{\epsilon^2 + 1} - \epsilon - t} + \frac{\sqrt{\epsilon^2 + 1} - \epsilon + 1}{4\epsilon^2} \frac{1}{\sqrt{\epsilon^2 + 1} + \epsilon + t} \right.$$

$$\left. -\frac{1}{4\epsilon} \frac{1}{1 - t} + \frac{\epsilon - 2}{4\epsilon^2} \frac{1}{1 + t} + \frac{1}{2\epsilon(1 + t)^2} \right\} \tag{A3}$$

A further substitution

$$t = \frac{\epsilon\sqrt{1 + \epsilon^2 + 2j^2}}{\epsilon + j^2} \sin\varphi - \frac{\epsilon^2 + j^2}{\epsilon + j^2} \tag{A4}$$

and treating the curly bracket in eq. (A3) term by term reduces the integral to the form

$$I_< = \frac{\hbar R_0^2}{\pi} \left\{ \sum_{i=1}^3 C_i J_>(A_1, a_i, b_1) + C_4 J_<(A_1, a_4, b_1) \right.$$

$$\left. + C_5 K_<(A_1, a_4, b_1) \right\} \tag{A5}$$

with the functions $J_<$, $J_>$, $K_<$ defined in eq. (4.37)–(4.38) and the parameters and coefficients given in eqs. (4.40)–(4.52).

Turning to the second part $I_>$ of I_r we may apply a similar sequence of substitutions resulting in

$$\rho = \sqrt{\frac{\epsilon + 1}{2} + \sqrt{\left(\frac{\epsilon + 1}{2}\right)^2 - j^2} \sin\varphi} \tag{A6}$$

which brings $I_>$ to the form

$$I_> = \frac{\hbar R_0^2}{\pi} C_6 J_>(A_2, a_5, b_2)$$

with the parameters and coefficients given in eqs. (4.40)–(4.52). From $I_r = I_< + I_>$ we obtain the result given in eq. (4.39).

APPENDIX B: NORMALIZATION OF THE WKB WAVE FUNCTION

Here we summarize the necessary steps in the evaluation of the integral in eq. (5.3). For type A motion the radial period is simply π/ω_0. To evaluate eq. (5.3) also for type B motion we introduce scaled variables like in eq. (4.6), and the integral is splitted in a part I_1 from $\rho_<$ to 1 and a part I_2 from 1 to $\rho_>$.

$$I_1 = \frac{1}{m\omega_0} \int_{\rho_<}^{1} d\rho \frac{\epsilon}{\sqrt{\epsilon^2 + (1-\rho^2)^2}} \frac{1}{\sqrt{-\left(\frac{j^2}{\rho^2} + 1 - \rho^2\right) + \sqrt{\epsilon^2 + (1-\rho^2)^2}}} \tag{B1}$$

$$I_2 = \frac{1}{m\omega_0} \int_{1}^{\rho_>} d\rho \frac{1}{\sqrt{\epsilon + 1 - \frac{j^2}{\rho^2} - \rho^2}} . \tag{B2}$$

A series of substitutions amounting to

$$\rho^2 = \frac{1 - t^2 - 2\epsilon t}{1 - t^2}$$
$$t = \left[\epsilon\sqrt{1 + \epsilon^2 + 2j^2} \sin\varphi - \epsilon^2 - j^2\right]/(\epsilon + j^2) \tag{B3}$$

puts I_1 into the form

$$I_1 = \frac{\epsilon\sqrt{\epsilon + j^2}}{m\omega_0} \int_{A_1}^{\pi/2} \frac{d\varphi}{\epsilon + \epsilon^2 + 2j^2 - \epsilon\sqrt{1 + \epsilon^2 + 2j^2}\sin\varphi} \tag{B4}$$

where A_1 is defined in (4.40). The integral is now elementary and given by

$$I_1 = \frac{2\epsilon}{\sqrt{2(\epsilon^2 + 2j^2)}} \frac{\beta}{m\omega_0} \tag{B5}$$

with β given by eq. (5.5). Here we used the addition theorem for arctan to simplify the final expression.
I_2 is much simpler to evaluate. The substitution

$$\rho^2 = \frac{\epsilon + 1}{2} + \sqrt{\left(\frac{\epsilon + 1}{2}\right)^2 - j^2} \sin\varphi \tag{B6}$$

reduces it to the form

$$I_2 = \frac{1}{2m\omega_0} \int_{A_2}^{\pi/2} d\varphi \tag{B7}$$

where A_2 is defined in eq. (4.41). After some simplification the result takes the form

$$I_2 = \frac{1}{2m\omega_0} \left(\frac{\pi}{2} - \alpha\right) \tag{B8}$$

with α given by eq. (5.5). Combining the results (B5), (B8) with eq. (5.3) we obtain eq. (5.4).

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FIG. 1. Regions of type A motion and type B motion in the scaled angular momentum-energy $(j - \epsilon)$-plane. In region D there is no lower turning point of the radial motion, i.e., in the semiclassical quantization region D is forbidden.

FIG. 2. Difference $\delta = \delta_n(\ell)$ of quasi-particle energy levels, in units of $\hbar\omega_0$, to the levels of the free trap. The chemical potential was chosen to be $\mu = 4.27\hbar\omega_0$.

FIG. 3. Dynamic structure function $S^{(1)}(k, \omega)$ in units of $d_0/a\hbar\omega_0$ for $\mu/\hbar\omega_0 = 4.27$, $kd_0 = 15.1$ as a function of ω in units of ω_0. Plotted are the strengths of the Dirac-delta peaks.

FIG. 4. Dynamic structure function $S^{(1)}(k, \omega)$ in units of $d_0/a\hbar\omega_0$ for $\mu/\hbar\omega_0 = 5.62$, $kd_0 = 3$ as a function of ω in units of ω_0. Plotted are the strengths of the Dirac-delta peaks. Peaks with equal principal quantum number $n = 2n_r + \ell$ are connected by straight lines, with $n = 9, 8, 7$ from top to bottom.

FIG. 5. Semiclassical selection rule 6.21 and semiclassical energy levels $E = E_{n_r\ell}$ in the (ℓ, E)-plane for $\mu/\hbar\omega_0 = 5.62$, $kd_0 = 3$.

FIG. 6. Dynamic structure function $S^{(1)}(k,\omega)$ in units of $d_0/a\hbar\omega_0$ for $\mu/\hbar\omega_0 = 13.1$, $kd_0 = 2$ as a function of ω in units of ω_0. Plotted are the strengths of the Dirac-delta peaks. Peaks with equal principal quantum number $n = 2n_r + \ell$ are connected by straight lines, with $n = 8, 7, 6$ from top to bottom.